ABSTRACT OF THE DISCLOSURE

The present invention provides for a method for validating a computer modeling of a molecular system. The method has the steps of selecting a model parameter of the molecular system; selecting a validation measure of the molecular system; simulating the molecular system by the computer modeling with the selected model parameter; then determining a value of the validation measure of said molecular system from the simulating step; and testing whether the value of the validation measure is in a predetermined range to validate the computer modeling. The method can be performed iteratively by varying the model parameter continuously, such as varying a temperature model parameter, or discretely, such as substituting for different residues in a protein.